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Induced ionization of small molecules: comparison of experiment with quantum and classical calculations

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Synopsis The ion-impact induced ionization of small molecules was investigated both experimentally and theoretically. Electron energy spectra were taken by an energy dispersive electrostatic spectrometer at different observation angles. The obtained absolute electron emission cross sections were compared with the results of CDW-EIS and CTMC calculations. Both theories are in a reasonable agreement with the experimental data.

Ionization of atoms and molecules is of fundamental interest in atomic and molecular physics [1,2]. Besides that, ionization is important in many applications, for instance plasma physics, industrial irradiations and radiotherapy. It was discovered recently that free electrons are almost as effective as free radicals in causing DNA damage in living cells [3].

In the experiment H^+, He^+, C^+ and N^+ ions were provided by a 5 MV VdG accelerator in the 46-1000 keV/u energy range. The ion beams crossed gas jets of CH_4, H_2O and N_2. By applying a rotatable energy dispersive electrostatic spectrometer we determined double differential electron emission cross sections (DDCSs) in the 20°-160° observation angle range. In figure 1 we compare the energy spectrum of the electrons ejected in 1 MeV H^+ + CH_4 collisions at 90° observation angle with CTMC and CDW-EIS [4] calculations.

In the CTMC calculations we used a multi-center three-body approach. Our model is very similar to that of Illescas et al. [5] except that we considered the full three-body dynamics. A very good agreement was found between the experimentally observed DDCS and that obtained by the CTMC calculations in the entire electron energy range. This indicates that the classical trajectory method can be applied for calculation of the ionization properties of few atomic molecules by bare projectiles in this intermediate collision energy range (see Fig. 1).

Above ~12 eV electron energy the quantum mechanical CDW-EIS calculations also show a good agreement with the experiment, the two theories practically agree. Below 10 eV both theories overestimate the experimentally obtained DDCSs, but CTMC only slightly.

Similarly, good agreement was observed between the measurement and the theories for all studied observation angles. According to the calculations, single ionization is dominant for the studied collision system. For such small perturbation, both theories seem to be adequate for treating the electron emission process from small molecules.

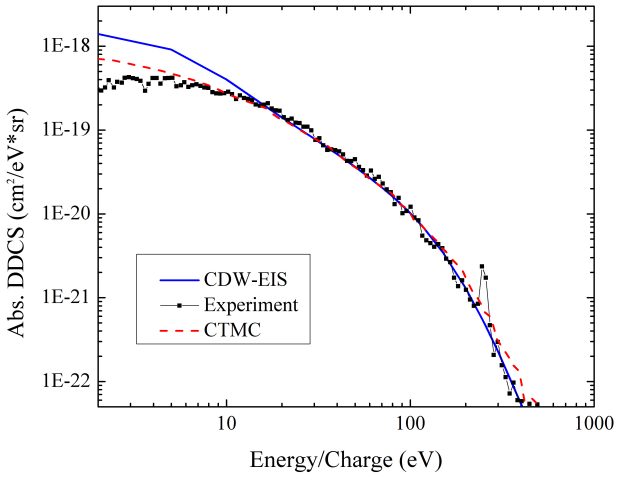

Figure 1. Comparison of the experimental electron spectrum with the results of CTMC and CDW-EIS calculations at 90° observation angle for 1 MeV H^+ + CH_4 collisions.

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